Computational Material Modeling of Hydrated Cement Paste Material Chemistry Structure – Influence of Magnesium Ion Exchange

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ABSTRACT

Cementitious materials have material, geometric features ranging from molecular/nano, micro-, meso- and macro scales. Features and changes in material chemistry/nano scale influence the hydration process, formed micro scale morphology, associated properties and behavior at engineering length scales. In the present paper, effect of material ion exchange on mechanical properties and shear deformation behavior of nano level hydrated cement constituent - calcium silicate hydrate (CSH) based on its material chemistry structure are studied following a molecular dynamics (MD) computational modeling methodology. Calcium ions are replaced with Magnesium ions in the traditional CSH-Jennite crystal structure [1] of the hydrated cement constituent. Traditional CSH-Jennite structure, and Magnesium modified structures obtained by calcium exchange of magnesium are used in the MD based material modeling analysis. Extensive modeling analysis established optimal computational MD modeling parameters and molecular material sizes employed. Material modeling for shear deformation was performed using a MD based shear deformation and failure analysis methodology developed in our research group [2]. The present study clearly shows the influence of material chemistry due to Magnesium ion exchange in CSH-Jennite with predicted elastic modulus changing as amount of Magnesium in CSH-Jennite material chemistry structure varies. The variations in shear stress-strain deformation behavior due to the magnesium ion exchange compared to traditional CSH are studied and discussed. This paper demonstrates that molecular material modeling methodology employed based on material chemistry is a viable approach to understand, computationally predict changes in mechanical properties, and deformation behavior due to material chemistry/nano level changes in cementitous materials. Shear deformation stress-strain behavior obtained through material chemistry level modeling of traditional and Magnesium modified CSH-Jennite showed the influence of magnesium ion exchanges on the onset of failure. Molecular deformation in the material chemistry level structures were analyzed and molecular level changes that clearly identified on-set of failure and influence of the material chemistry ion-exchages on computationally predicted stress-strain behavior and molecular level failure are discussed and presented.

REFERENCES

[1] I. G. Richardson, "Tobermorite/Jennite and tobermorite/calcium hydroxide based models for the structure of CSH: Applicability to hardened pastes of tricalcium silicate, β dicalcium silicate, Portland Cement, and blends of Portland cement with blast-furnace slag, metakaolin, or silica fume", *Cement and Concrete Research*, **34**, 1733-1777 (2004).

[2] J. S. Murillo, A. Mohamed, W. Hodo, R, V. Mohan, A. Rajendran, R. Valisetty, "Computational Modeling of Shear Deformation of Nanoscale Hydrated Calcium Silicate Hydrate (CSH) in Cement Paste: CSH Jennite, *Int. J. Damage Mechanics- Special Issue on Failure of Nano, Bio, and Micro Materials*, submitted (2014).